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Title: Monte Carlo Approaches for Uncertainty Quantification of Criticality for System Dimensions

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Monte Carlo Approaches for Uncertainty Quantification of Criticality for System Dimensions

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Abstract

MCNP6 is used to estimate uncertainties from geometric tolerances using forward and adjoint methods. Results are obtained and the forward and adjoint approaches appear to agree in some cases where the responses are not non-linearly correlated. In other cases, the uncertainties in k disagree for reasons not yet known.

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Introduction

- Motivation
- Forward/Direct Approach
- Adjoint/Perturbation Approach
- Results

Motivation

- Experimental benchmark uncertainty arises from many unknowns about the state of the experiment.
- Benchmark uncertainty must be known to create bias curves for validation.
- Geometric uncertainties from manufacturing tolerances, poor records, etc. may contribute significantly.
- This work focuses on two methods to quantify them:
  - Forward (brute force).
  - Adjoint (perturbation theory).

Forward Approach

- Let X be a vector of uncertain model parameters x_i.
- Each x_i has an underlying random distribution $f_i(x_i)$ (e.g., uniform, normal, etc.) and may be correlated with other parameters x_j.
- Procedure:
    - Randomly sample N independent realizations of $f_i(x_i)$.
    - Generate input files, run transport calculations, compute k for each.
    - Use sample statistics to find empirical <u>population</u> standard deviation on distribution of k to estimate uncertainty δk.

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mcnp_pstudy

- Preparing numerous input files by hand is a very cumbersome process on the part of the analyst.
- Fortunately, MCNP provides a utility script, *mcnp_pstudy* to greatly simplify the workflow.

- Analyst creates a special (master) MCNP input file with macros that can be random variables with constraints.
- *mcnp_pstudy* processes the master input file, producing many separate inputs, runs MCNP on each, and collects results.
- Perl source provided with MCNP distribution, so advanced users can modify to meet their needs.

Forward Approach

- Advantages:
  - Conceptually simple and *mcnp_pstudy* is fairly straightforward to use.
  - Capture general random distributions including non-linear correlation.
  - Produces correct result given model assumptions.
- Disadvantage:
  - May be very computationally expensive for multidimensional parameter variations.
  - Not an issue if you have a cluster, but may be prohibitive for those with a single workstation.

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Adjoint/Perturbation Approach

- Perturbation theory may be applied to find derivatives of k with respect to system parameter x.
- Given derivatives, apply the "sandwich rule" to estimate uncertainty:

$$(\delta k)^2 = \mathbf{SCS}^T.$$

- $\mathbf{S}$ is a vector of sensitivities (derivatives).
- $\mathbf{C}$ is the covariance matrix.

Adjoint/Perturbation Approach

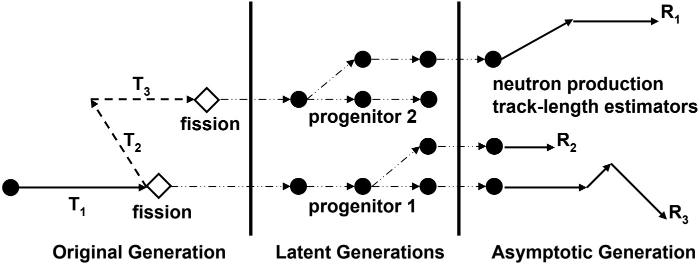
- For a uniform expansion/contraction about boundary B:

$$\frac{dk}{dr} = \frac{1}{M}\Big[\left\langle \psi^\dagger, \left(\Sigma_t^+ - \Sigma_t^-\right)\psi \right\rangle_B + \left\langle \psi^\dagger, S^-\psi \right\rangle_B - \left\langle \psi^\dagger, S^+\psi \right\rangle_B + \left\langle \psi^\dagger, \lambda F^-\psi \right\rangle_B - \left\langle \psi^\dagger, \lambda F^+\psi \right\rangle_B \Big].$$

- $\psi^\dagger$ is the adjoint/importance function.
- M is the adjoint-weighted fission source, S is the scattering operator, and F is the fission operator.
- Integrals are over surface defining boundary B.
- $+$ and $-$ terms represent the material on the respective positive and negative sides of the surface (w.r.t. surface normal).

Computing Adjoint-Weighted Integrals

- Divide active cycles or generations into "blocks" of some size (default 10).
- First cycle: accumulate scores for forward reaction rates and tag neutrons.
- Follow neutrons through generations, preserving tags.
- Last cycle: multiply forward reaction rates by neutron production of corresponding progeny.



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Computing Adjoint-Weighted Integrals

- At each surface crossing, must create artificial neutrons to have scattered or been emitted by fission at boundaries with both $+$ and $-$ materials.
- These are followed through generations and used only to weight surface flux—not involved in other tally scores.
- May be computationally resource intensive. Perhaps this could be approximated with a precomputed surface-based Green's function.

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Adjoint/Perturbation Approach

- Advantages:
  - Often times much less computationally costly than direct approach.
  - Easy user interface (specify list of surfaces that are uncertain).
- Disadvantage:
  - Approximate (linear perturbation) and limited to normal distributions with linear correlation.

Test Problems

- Bare Pu Cylinder
  - Case 1: Perturb radius R and height H independently (normal distribution).
  - Case 2: Perturb R and H to preserve mass (non-linear correlation).

- Case 3: Pu Nitrate Cylinder in Stainless Steel Can
  - Perturb volume of solution, inner can radius, and can thickness independently (normal distribution).
  - Model parameters: Solution height H_{sol}, inner radius R_{in}, and outer radius R_{out} are correlated, however.

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Results: Bare Pu Cylinder

- Uncertainty δk in pcm for cases 1 and 2.

	Forward	Adjoint	C/E
Case 1	4126	4277	1.037
Case 2	852	938	1.101

- Reference is the Forward result.
- Case 1 agrees within 1-2σ.
- Case 2 disagrees by more than 3σ; expected because adjoint method cannot capture non-linear correlation.
- Still within 10% (may be acceptable), and obtained in minutes versus hours of CPU time.

Results: Case 3 (Pu Nitrate Solution)

- Need a linear estimate of (non-linear) correlation matrix.
- Obtain empirically by direct sampling with *mcnp_pstudy*:

	R_{in}	R_{out}	H_{sol}
R_{in}	0.104	0.984	-0.352
R_{out}	0.984	0.106	-0.363
H_{sol}	-0.352	-0.363	2.120

- Diagonal is standard deviations (cm).
- Off-diagonal is linear (Pearson) correlation coefficients.

Results: Case 3 (Pu Nitrate Solution)

x_i	dk/dx_i (cm^{-1})	δk (pcm)
R_{in}	-4.524×10^{-2}	475
R_{out}	6.460×10^{-2}	688
H_{sol}	1.156×10^{-3}	245
Correl.		-585
Adjoint		274
Forward		663

- Large disagreement. Adjoint model likely inappropriate.
- Sensitivities also show disagreement; may indicate error in method, although similar cases in other work show agreement.

Summary

- Demonstrated forward and adjoint approaches for geometric uncertainty quantification.
- Forward result works and is straightforward to use with *mcnp_pstudy*, but it is computationally expensive.
- Adjoint methods can show poor agreement; investigation continues.

Acknowledgments

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Questions?